# A Study of Carbon Monoxide Distribution Determinations for a Global Transport Model

Final Report

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## Introduction

The first MAPS (Measurement of Air Pollution from Satellites) experiment was conducted on OSTA-1 in the payload bay of the space shuttle during November 1981. The purpose of the experiment was to measure the carbon monoxide concentration in the middle and upper troposphere. The instrument took approximately 10,000 measurements that were ultimately satisfactory for data reduction.

The results of the OSTA-1 experiment had a precision of 20%. The carbon monoxide concentration, as determined by MAPS, was dependent on both latitude and longitude with the lowest concentrations in the Southern Hemisphere. Several regions of high concentration could be identified. Comparison of one such region over northern South America with model predictions helped to partially validate the results of the experiment. See Reichle, et al. (1986) for more details.

A complete validation of the MAPS experiment is a crucial factor to ascertain the significance of the data for both OSTA-1 and OSTA-3, and to assist in improving the instrument before future missions if necessary. Now that the data from OSTA-1 have been analyzed, various projects have been identified which can indicate carbon monoxide trends, validate the experiment, and improve present models. The success of the previous missions has required the MAPS research group to spend considerable time on data reduction and preparing the instrument for future flights. Therefore, many of the projects that are of scientific interest have not been attempted. One option is for MAPS Science Team researchers and their colleagues to pursue these projects to assist the primary research group.

The primary objective of this grant was to further the development of a global transport/chemistry model that simulates the physico-chemical behavior of methane and carbon monoxide in the troposphere. The computer simulation

model is designed to analyze the processes that occur as methane and carbon monoxide are transported from their respective sources to their ultimate fate, e.g., final conversion to $CO_2$, transport to the stratosphere, deposition at ground level, etc.

## Model Description

The model predictions for carbon monoxide and methane require three separate models: mass consistent model, which calculates vertical winds from the horizontal wind field (Kitada, et al., 1983); boundary layer model, which calculates the height of the boundary layer and eddy diffusivities (Mellor and Yamada, 1974 and Yamada and Mellor, 1975); and global transport model, which simulates the chemistry and movement of CO and $CH_4$ in the atmosphere (Kitada and Peters, 1982).

The system of programs which model the chemistry and transport of carbon monoxide and methane in the earth's troposphere on a global scale has been installed on the NASA-Langley central scientific computer network, the IBM 3090-300E at the University of Kentucky, and the CYBER 205 at GFDL/NOAA at Princeton University. This system, the GLOBAL system, consists of a user-friendly set of procedural files which allow for simplified pre-processing, execution, and post-processing for all program elements. The package includes procedures for obtaining the NMC meteorological data, calculating the vertical winds to satisfy mass conservation, determining the boundary layer, and executing the transport/chemical model for carbon monoxide. In addition, plotting, saving to tape, and reading from tape routines have been developed.

Final modifications to the sub-programs for processing the input data for the transport/chemistry model have improved these data to more accurately

reflect true atmospheric conditions. The growth and decay of the boundary layer corresponds to the solar zenith angle. Notwithstanding boundary conditions, mass conservation is within the requirements of the transport/chemistry model; e.g., the characteristic time for the divergence term is greater than the integration time step of the model.

The transfer of the transport/chemistry model from the NCAR CRAY system to the NASA-Langley VPS-32 system was completed; however, several formerly unrecognized complications emerged. Initial modifications to input and manipulate actual meteorological data proved ineffective. These problems were traced to system idiosyncrasies and erroneous automatic vectorization. The source data for carbon monoxide and methane were originally stored on magnetic tape at NCAR. With multiple system changes, these data were lost and it became necessary to re-enter the data from original listings.

Several minor, but significant, errors in the computer algorithm were identified and corrected during the course of installing the transport/chemistry model onto the VPS-32 computer. The most perplexing of these errors was an incorrectly modified matrix solver. This subroutine correctly solved the matrix for a uniform wind field as had been used in previous operational runs; however, when the actual meteorological data were input, the subroutine could not correctly solve the matrix. Replacing this subroutine with a library routine proved to be an easy solution for this problem.

With these problems eliminated, progress toward complete installation led to two further difficulties: (1) the degree that mass conservation is maintained during temporal interpolations may not be within the limits of the model requirements; and (2) the boundary conditions at longitude $180^{o}$ West appeared not to correctly account for the correct mass flow.

Various test cases were completed where the chemistry and transport were separately and jointly suspended. These cases provided a basis for determining the cause of the errors. Further studies of the transport/chemistry model were accomplished at the University of Kentucky and at GFDL/NOAA.

## Model Structure

The attached flowcharts indicate the sequence of procedures which are executed for each twelve-hour period of meteorological data. The system is controlled by the main procedure named GLOBAL. The user is prompted for the program step which is to be executed. Automatic execution of the entire system could be attempted; however, a system malfunction could cause undetectable or costly errors. GLOBAL attaches and executes the appropriate procedure for the user-selected program.

The meteorological data must be processed by four FORTRAN programs: METRLGY for retrieving a subset ($5^{o}$ x $5^{o}$ grid) of the packed metrological data; WINDFLD for calculating the vertical wind field ensuring mass conservation; BOUNDRY for determining the vertical eddy diffusivities and interpolating the meteorological data over a twelve-hour period; and TRANSPT for simulating the transport and chemistry model for carbon monoxide and methane. In addition, a fifth program, INITIAL, initializes the source and terrain data for the system.

As indicated in the flowcharts, each sub-system requires multiple job files to process the input and output files and queue the programs for execution on the appropriate computer. These job files have the following suffixes and function. The -PRC procedural file prompts the user for the date and hour for which the program will be executed and creates a -DAT file for input into the program. For the VPS-32 system, the -JOB job file routes the

corresponding job file to that computer except for the METRLGY sub-system where the -JOB job file actually queues and controls this program. The -VPS job file queues and controls the execution of the four VPS-32 programs. And finally, the -SUB job file queues the output files for printing.

For each twelve-hour period, six output files are generated by the GLOBAL system: MDATA, which contains the NMC meteorological data from the METRLGY program; WDATA, which contains the results of the WINDFLD program; BDATA, which contains the results of the BOUNDRY program; KDATA, which contains the eddy diffusivities for the next time step of the BOUNDRY program; CDATA, which contains the carbon monoxide and methane for the next time step of the TRANSPT program; and TDATA, which contains the final results of the TRANSPT program.

The model has been run for one time step at GFDL/NOAA, Princeton University on a CYBER 205. The programs were loaded on a front-end CYBER 170 as data files. Using appropriate job procs available at GFDL, libraries containing the source decks of the various programs were created.

The original programs had special machine-specific calls to perform I/O. In order to make the GLOBAL package portable to other machines, these I/O calls were replaced by standard FORTRAN 77 read and write statements. All reads now occur from units 11 to 20, while output files are written to units 21 to 30. Diagnostic print files are written to unit 51.

The programs were compiled using a FORTRAN 77 compiler. Rundecks were created to run the programs as batch jobs. Certain compiler and run-time errors were discovered which were corrected. The following changes were made to the program WIND: a) U0, V0, T0, Z0, and R0 were read in before the calculation of $dz_o/dx$ and $dz_o/dy$; b) UC and VC at $\rho$ = NZ were defined similar to the definition at $\rho$ = 0; and c) the bottom level was changed from $\rho$ = 0.0167 to $\rho$ = 0.0. In addition, the following changes were made to the program BOUN: a) TEM2(L2lMl) was changed to TEM2(LNX,LNY,L2lMl); b) 2 right

parantheses were adjusted in the QL calculation; and c) statements numbered 9090 and 9100 were moved inside the IF block.

A coding error was discovered in the subroutine SOLPHI. This subroutine solves the almost-triadiagonal system of equations obtained from the $\phi$ - direction governing differential equation. The subroutine was corrected and tested by solving a problem involving the pure rotation of a wedge-shaped initial distribution.

The program TRAN was run for a single time-step to ensure that the program flow was correct. The CPU time for this run was approximately 80 seconds on the CYBER 205. An analysis program, ANAL, was written to read the output files generated by TRAN. This was run successfully to print diagnostic information in a tabular form.

In Appendix A, instructions to run the GLOBAL package are presented. The final program files have also been downloaded onto IBM-PC diskettes for easy transfer to other systems.

## REFERENCES


Kitada, T., A. Kaki, H. Ueda, and L. K. Peters, Estimation of vertical air motion from limited horizontal wind data - a numerical experiment, **Atmos. Environ., 17,** 2181-2192, 1983.

Kitada, T. and L. K. Peters, A three dimensional transport-chemistry analysis of CO and $CH_4$ in the troposphere, Second Symposium on the Composition of the Nonurban Troposphere, 96-101, 1982.

Mellor, G. L. and T. Yamada, A hierarchy of turbulence closure models for planetary boundary layers, **J. Atmos. Sci., 31,** 1791-1806, 1974.

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Appendix A

Instructions for Running the GLOBAL Package

NOTE: In all cases, open and close statements should be inserted in the programs to associate unit numbers with corresponding data files.

1. Run program INIT. This program puts source, terrain, initial concentration, and initial eddy diffusivity data in a format readable by TRAN. There are two input files: ISOURCE.GBL and ITERAIN.GBL. These should be associated with units 11 and 12, respectively. Output files are IPDATA (unit 51), TERRAIN (unit 21), SOURCES (unit 22), KDATA (unit 23), and CDATA (unit 24).

2. Run program METR. This program reads the NMC data tape (unit 11) and extracts u, v, $\rho$, T, and geopotential height data corresponding to a particular time. The time is specified in input file METDAT (unit 12 - user supplied), which is a NAMELIST input file containing the year, month, day, and hour of the start of the 12 hour simulation. METRLGY should be run twice by changing METDAT to extract data at the start and end of the 12 hour period of interest. The corresponding output files are MDATA1 and MDATA2 (unit 21) and MPDATA1 and MPDATA2 (unit 51).

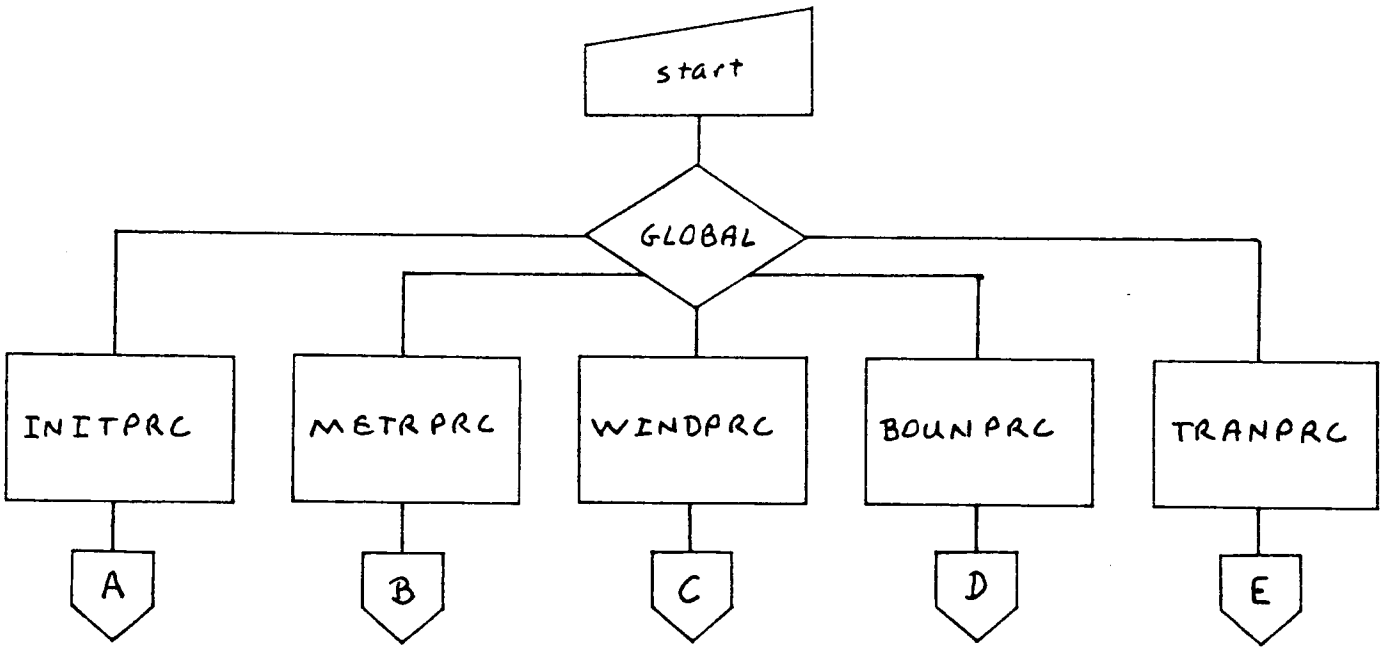
3. Run program WIND. This program interpolates meteorological data to 9 pre-specified levels. This program should also be run twice using MDATA1 and MDATA2 (unit 11) as input files to generate output files WDATA1 and WDATA2 (unit 21), respectively. Other input files are WINDAT (unit 12 - user supplied NAMELIST input file containing time of start of simulation)

and TERRAIN (unit 13). Print files MPDATA1 and MPDATA2 (unit 51) are also generated as output.

4. Run program BOUN. This program generates meteorological data at 30 minute intervals. Input files are BOUNDAT (unit 11 - user specified data file), WDATA1 (unit 12), WDATA2 (unit 13), and TERRAIN (unit 14). Output files are BDATA (unit 21), and BPDATA (unit 51).

5. Run program TRAN. This is the transport/chemistry code. Input files are TRANDAT (unit 11 - user specified data file), CDATA (unit 12 - from INIT on first run and then from TRAN on subsequent runs), SOURCES (unit 13), WDATA1 (unit 14), and BDATA (unit 15). Output files are CDATA (unit 21), and CPDATA (unit 51).

6. Run program ANAL. This program reads CDATA files at start and end of 12 hour integration period (units 11 and 12, respectively), and WDATA1 (unit 13) and generates ADATA (unit 51).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INITPRC
METRPRC
WINDPRC
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TRANPRC
A
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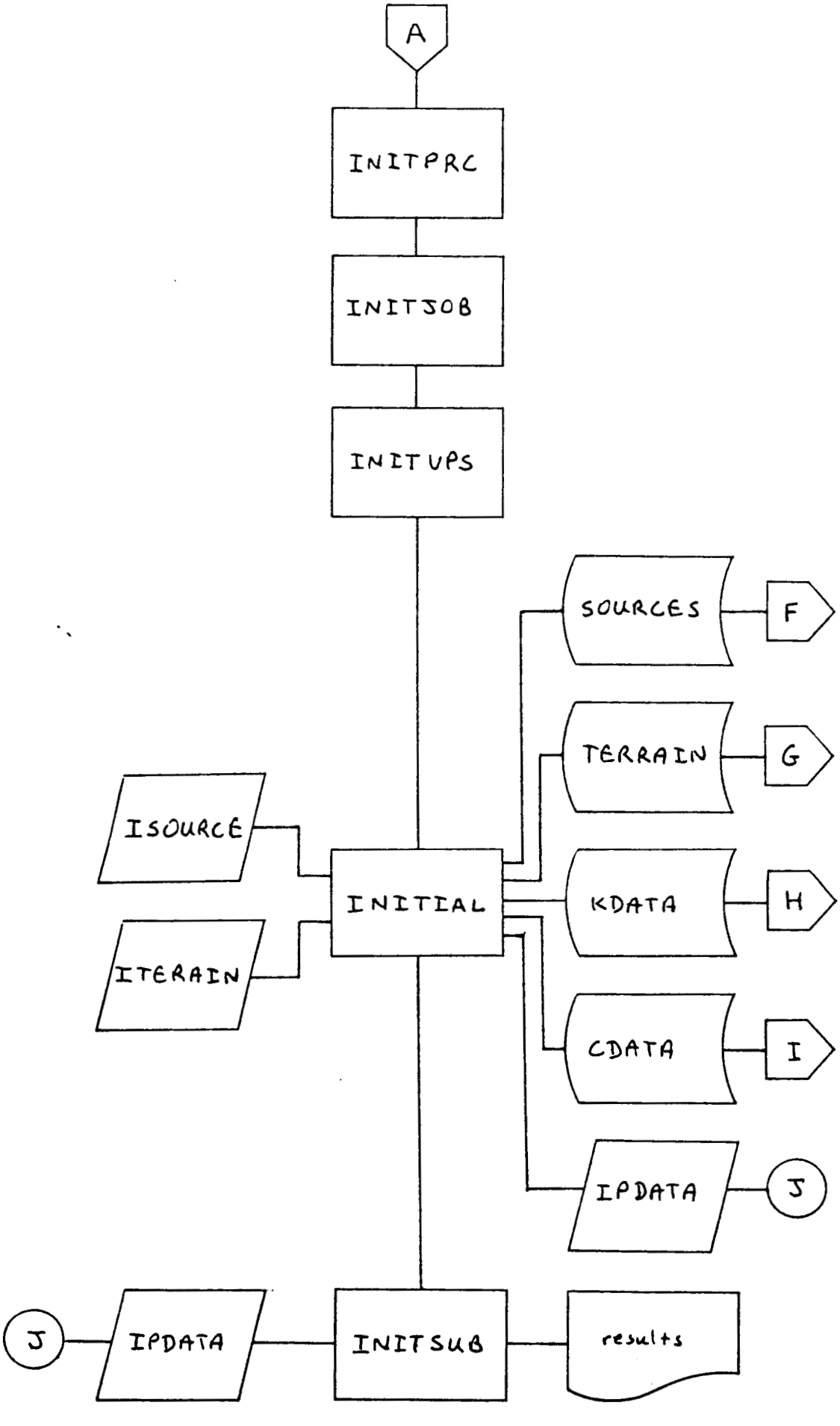
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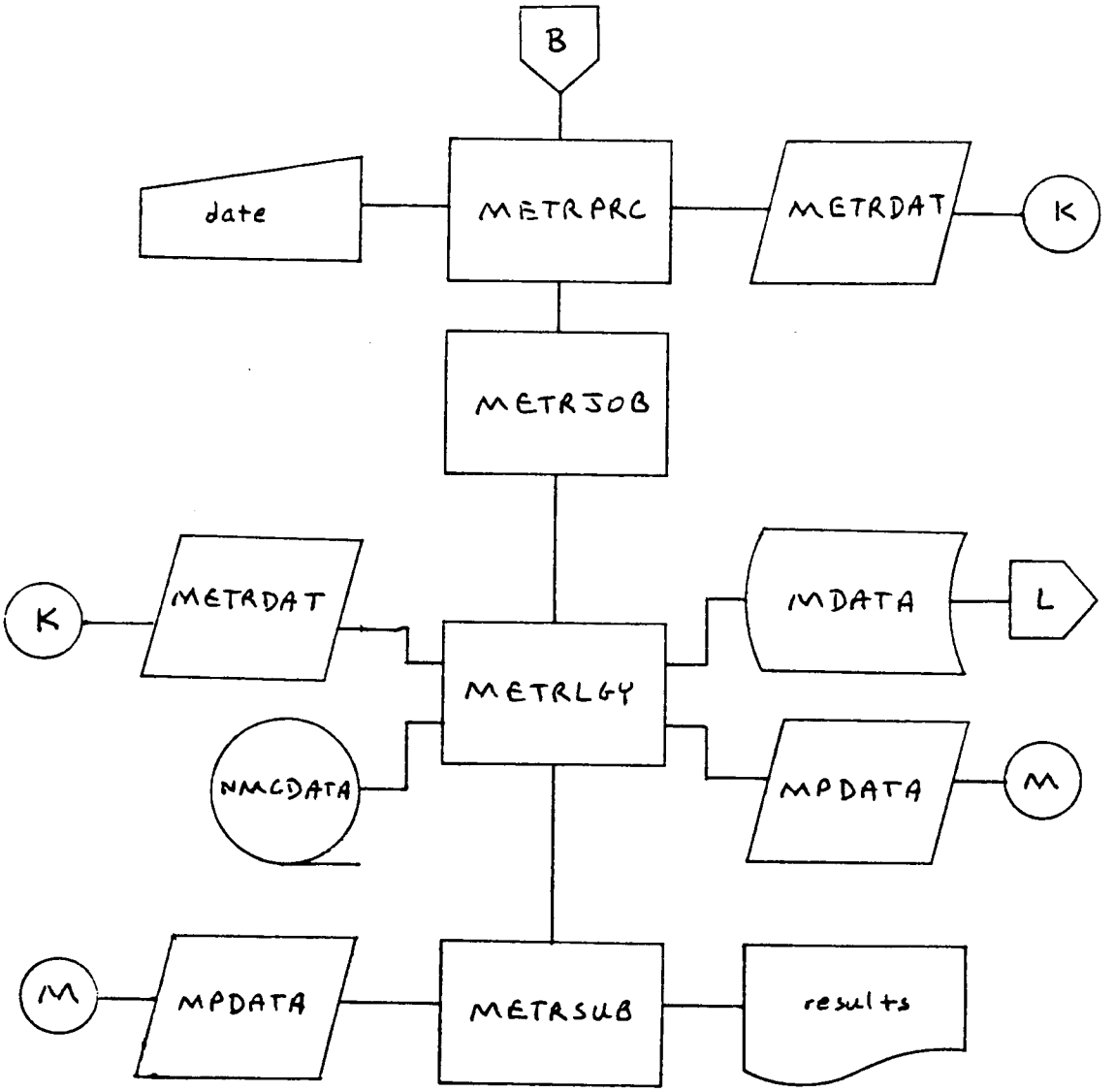
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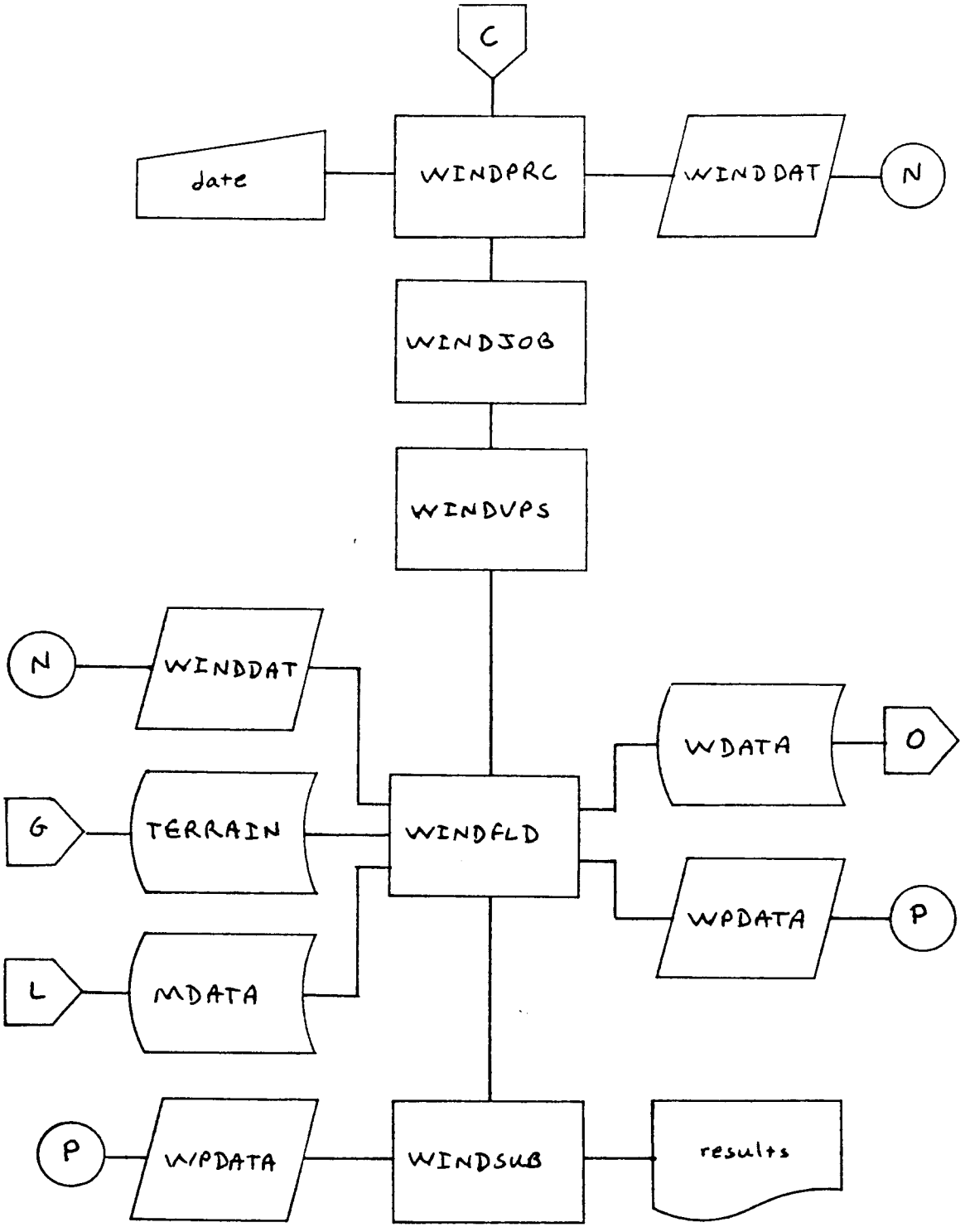
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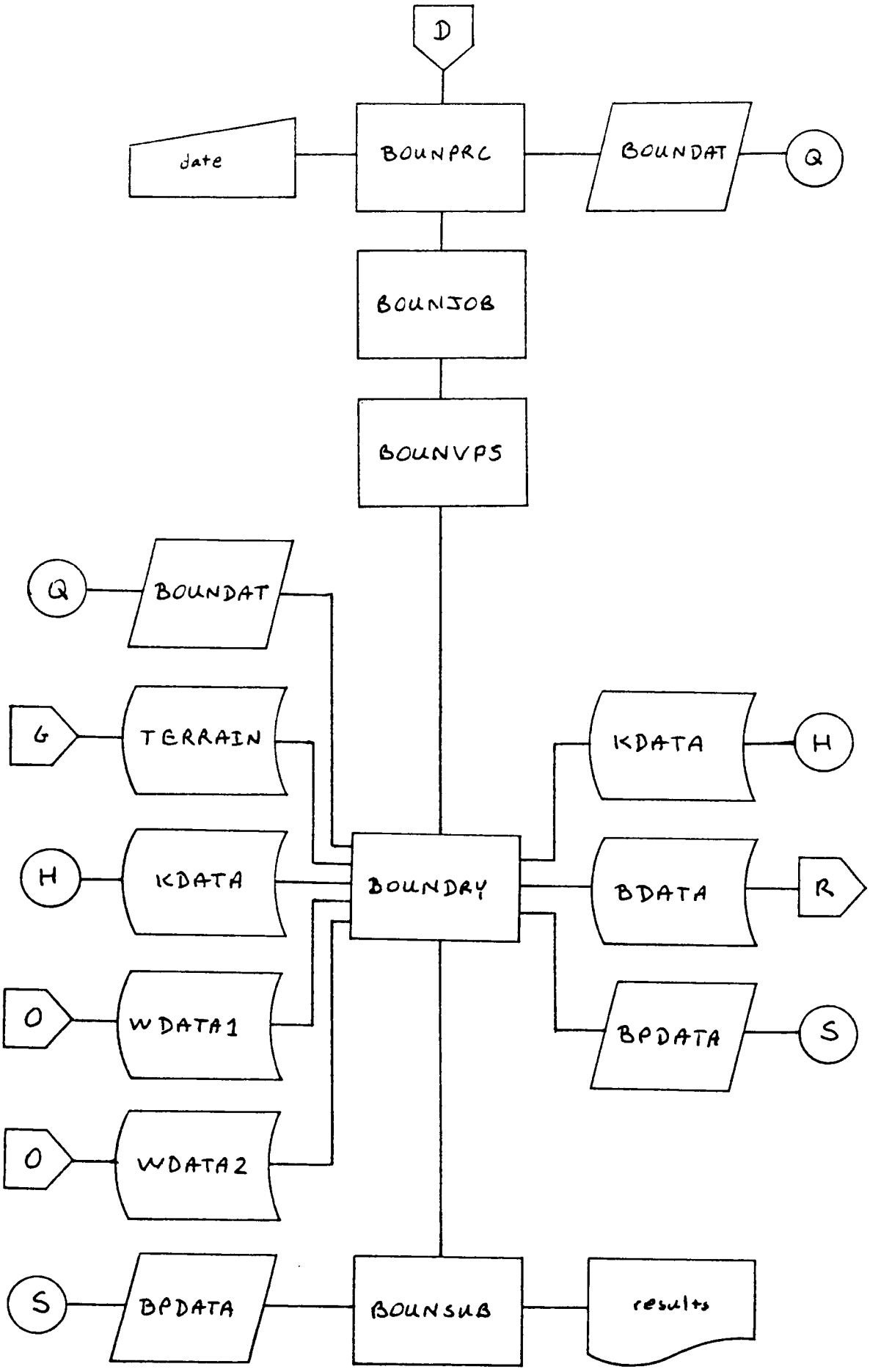
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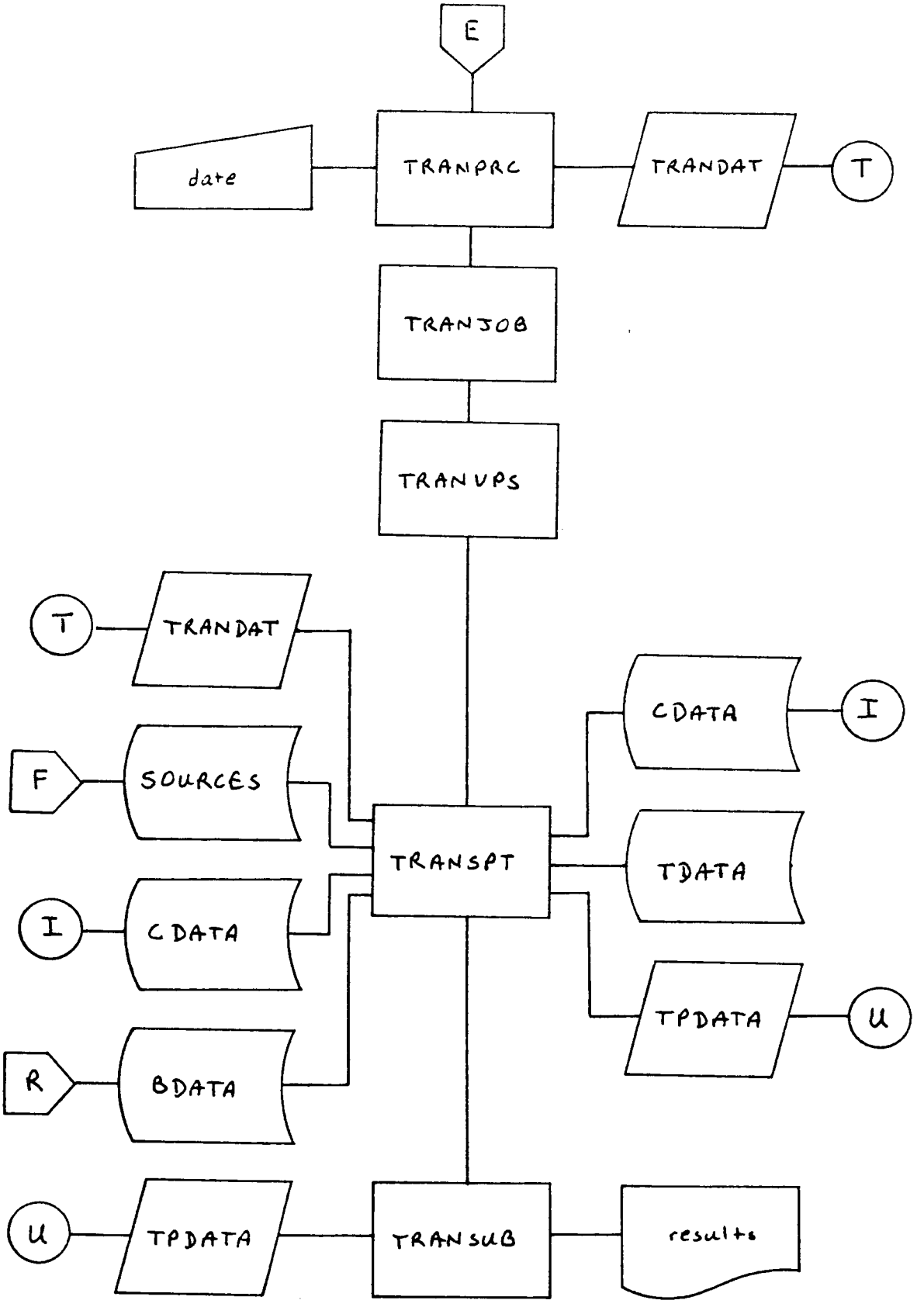
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